

# Exchange effects in plasmas: the case of low-frequency dynamics

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Recently, there has been a surge in the interest of non-equilibrium collective quantum models, where particle dispersion and spin are examples of effects taken into account. Here, we derive a kinetic plasma model containing fermion exchange effects. Exchange interactions are of great importance in many systems, and have no classical analogy. Our model therefore constitute a possible probe of collective quantum phenomena in new regimes. As an example, we consider the influence of exchange effect on low frequency dynamics, in particular ion acoustic waves. Comparisons to related computational techniques are given and the differences are highlighted. Furthermore, we discuss the applicability of our model, its limitations and possible extensions.

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Quantum plasma physics is currently a field of intense study. One reason for this is the potential applications in, for example, laser produced plasmas, ultra small electronic devices, and dense astrophysical systems [1–3]. Different aspects of quantum plasmas have been studied such as quantum dispersion and Fermi pressure [1–3], the magnetic dipole force and the spin dynamics [4–13], quantum relativistic effects and nonlinear dynamics [10–12, 14, 15]. Typically, quantum effects are important for systems with high density and low temperature. This said, it is important to distinguish between quantum effects related to thermodynamic equilibrium properties and dynamical properties of the system. Exchange effects due to particle statistics have been successfully included in the density functional theory (DFT) [16, 17]. Applications of DFT include for example ground state properties of atoms and equilibrium properties of many-particle systems via density functional theory [16, 17]. The effects of exchange on dynamics have also been studied in the setting of kinetic theory [4, 18–24], as well as in studying, e.g., the thermodynamic properties of plasmas [20, 21]. It has also been studied using fluid theory [24]. Furthermore, many papers deal with how quantum mechanics affects the low-frequency long-scale dynamics, as for example quantum ion acoustic waves [25–29].

In the present letter we have derived the quantum kinetic evolution equation for electrons within the Hartree-Fock approximation, treating the exchange effects perturbatively. The general result is further simplified by considering a plasma that is not spin-polarized, and by focusing on length scales much longer than the characteristic de Broglie length. We apply the formalism to one-dimensional ion-acoustic waves in plasmas, within the linear approximation.

We here consider a completely ionized electron-ion plasma with the particles interacting through a mean-field scalar potential. Quantum effects for the ions will be completely neglected, while for the electrons we will take into account a dynamic correction due to the Pauli exclusion principle. Also,

we will not consider effects due to the self-energy and particle correlations [21]. We will now give an outline of the derivation of a kinetic theory, where the exchange effect is taken into account.

The state of the  $N$ -electrons is described by the density operator  $\rho_{1\dots N}$  (see for example Ref. [21]), and the dynamics is given by the von Neumann equation with the Hamiltonian

$$\hat{H}_{1\dots N} = \sum_{i=1}^N \frac{\hat{p}_i^2}{2m_e} + \frac{e^2}{4\pi\epsilon_0} \sum_{i<j} \frac{1}{|\hat{\mathbf{x}}_i - \hat{\mathbf{x}}_j|} + e \sum_{i=1}^N \varphi(\hat{\mathbf{x}}_i). \quad (1)$$

Here  $m_e$  is the electron mass,  $e$  is the electron charge ( $e < 0$ ) and  $\epsilon_0$  is the permittivity of vacuum. The last term accounts for the interaction with the electric potential created by the ions. We now introduce the reduced density operators according to  $\rho_{1\dots i} = n^i \text{Tr}_{i+1\dots N} \rho_{1\dots N} \Lambda_{1\dots i}$ , where  $n$  is the mean density and  $\Lambda_{1\dots i}$  is the operator that takes an  $i$ -particle state and makes it completely antisymmetric. We will only need to know that  $\Lambda_{12} = 1 - P_{12}$  where  $P_{12}$  interchanges particle 1 and 2 (see, e.g., Ref. [21] for further details). The evolution for the one-particle density operator is given by

$$i\hbar \partial_t \rho_1 = [h_1, \rho_1] + n \text{Tr}_2 [V_{12}, \rho_{12} \Lambda_{12}], \quad (2)$$

where  $h_1 = \hat{p}^2/(2m_e)$  and  $V_{12} = V(\hat{\mathbf{x}}_1 - \hat{\mathbf{x}}_2) = q^2/(4\pi\epsilon_0|\hat{\mathbf{x}}_1 - \hat{\mathbf{x}}_2|)$  and  $\rho_{12}$  is the two-particle density operator. The effects of two-particle correlations  $g_{12}$  can be separated out of the two-particle density operator by writing it in the form  $\rho_{12} = \rho_1 \rho_2 + g_{12}$ . We are interested in the collisionless limit where a mean-field approximation will suffice. This approximation is obtained by neglecting the correlation function  $g_{12}$ . Utilizing this in the equation above we then get

$$i\hbar \partial_t \rho_1 = [h_1, \rho_1] + [\bar{V}_1, \rho_1], \quad (3)$$

where  $\bar{V}_1 = \text{Tr}_2 V_{12} \rho_2 \Lambda_{12}$ , is the Hartree-Fock potential. This is a closed system for the one-particle density operator. The evolution equation Eq. (3) can also be written in the Wigner representation, i.e.

$$\begin{aligned}
& \partial_t f(\mathbf{x}, \mathbf{p}, \alpha, \beta) + \frac{1}{m} \mathbf{p} \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{p}, \alpha, \beta) + \frac{ie}{\hbar} \int \frac{d^3 y d^3 p'}{(2\pi\hbar)^3} e^{i\mathbf{y} \cdot (\mathbf{p} - \mathbf{p}')/\hbar} \left[ \phi\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) - \phi\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \right] f(\mathbf{x}, \mathbf{p}', \alpha, \beta) \\
&= \frac{i}{\hbar(2\pi\hbar)^3} \sum_{\gamma=1}^2 \int d^3 p' d^3 p'' d^3 y d^3 r e^{i\mathbf{p} \cdot \mathbf{y}/\hbar} e^{-i\mathbf{p}' \cdot (\mathbf{x} + \mathbf{y}/2 - \mathbf{r})/\hbar} e^{-i\mathbf{p}'' \cdot (\mathbf{r} - \mathbf{x} + \mathbf{y}/2)/\hbar} \\
&\quad \times \left[ V\left(\mathbf{x} + \frac{\mathbf{y}}{2} - \mathbf{r}\right) - V\left(\mathbf{x} - \frac{\mathbf{y}}{2} - \mathbf{r}\right) \right] f\left(\frac{\mathbf{x} + \mathbf{r}}{2} + \frac{\mathbf{y}}{4}, \mathbf{p}', \alpha, \gamma\right) f\left(\frac{\mathbf{x} + \mathbf{r}}{2} - \frac{\mathbf{y}}{4}, \mathbf{p}'', \gamma, \beta\right), \tag{4}
\end{aligned}$$

where

$$f(\mathbf{x}, \mathbf{p}, \alpha, \beta) = \frac{n}{(2\pi\hbar)^3} \int d^3 y e^{i\mathbf{y} \cdot \mathbf{p}/\hbar} \rho\left(\mathbf{x} + \frac{\mathbf{y}}{2}, \alpha; \mathbf{x} - \frac{\mathbf{y}}{2}, \beta\right) \tag{5}$$

is the Wigner matrix for a spin-1/2 particle ( $\alpha, \beta = 1, 2$ , for spin up and down along the axis of quantization) and

$$\phi(\mathbf{x}) = \frac{en}{4\pi\epsilon_0} \sum_{\gamma=1}^2 \int d^3 z \frac{\rho(\mathbf{z}, \gamma; \mathbf{z}, \gamma)}{|\mathbf{x} - \mathbf{z}|} + \varphi(\mathbf{x}). \tag{6}$$

is the Wigner distribution and the total (mean-field and ex-

ternal) potential, respectively and  $V(\mathbf{x}) = q^2/(4\pi\epsilon_0|\mathbf{x}|)$  is the Coulomb potential. The LHS of Eq. (4) represents the quantum Vlasov equation, while the RHS is the correction due to exchange effects. This term is nonlocal in phase-space and nonlinear in the distribution function.

The matrix equation can be transformed into a scalar equation by taking the spin transformation [8]

$$f(\mathbf{x}, \mathbf{p}, \mathbf{s}, t) = \frac{1}{4\pi} \sum_{\alpha, \beta=1}^2 [\delta_{\alpha, \beta} + \mathbf{s} \cdot \boldsymbol{\sigma}_{\alpha, \beta}] f(\mathbf{x}, \mathbf{p}, \beta, \alpha), \tag{7}$$

where  $\mathbf{s}$  is a vector on the unit sphere. Applying this to Eq. (4) we obtain

$$\begin{aligned}
& \partial_t f(\mathbf{x}, \mathbf{p}, \mathbf{s}) + \frac{1}{m} \mathbf{p} \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{p}, \mathbf{s}) + \frac{ie}{\hbar} \int \frac{d^3 y d^3 p'}{(2\pi\hbar)^3} e^{i\mathbf{y} \cdot (\mathbf{p} - \mathbf{p}')/\hbar} \left[ \phi\left(\mathbf{x} + \frac{\mathbf{y}}{2}\right) - \phi\left(\mathbf{x} - \frac{\mathbf{y}}{2}\right) \right] f(\mathbf{x}, \mathbf{p}', \mathbf{s}) \\
&= \frac{i}{\hbar} \int \frac{d^3 p' d^3 p'' d^3 y d^3 r}{(2\pi\hbar)^3} e^{i\mathbf{p} \cdot \mathbf{y}/\hbar} e^{-i\mathbf{p}' \cdot (\mathbf{x} + \mathbf{y}/2 - \mathbf{r})/\hbar} e^{-i\mathbf{p}'' \cdot (\mathbf{r} - \mathbf{x} + \mathbf{y}/2)/\hbar} \int \frac{d^2 s' d^2 s''}{8\pi} [1 + 9\mathbf{s}' \cdot \mathbf{s}'' + 3\mathbf{s} \cdot (\mathbf{s}' + \mathbf{s}'') + 9i\mathbf{s} \cdot (\mathbf{s}' \times \mathbf{s}'')] \\
&\quad \times \left[ V\left(\mathbf{x} + \frac{\mathbf{y}}{2} - \mathbf{r}\right) - V\left(\mathbf{x} - \frac{\mathbf{y}}{2} - \mathbf{r}\right) \right] f\left(\frac{\mathbf{x} + \mathbf{r}}{2} + \frac{\mathbf{y}}{4}, \mathbf{p}', \mathbf{s}'\right) f\left(\frac{\mathbf{x} + \mathbf{r}}{2} - \frac{\mathbf{y}}{4}, \mathbf{p}'', \mathbf{s}''\right), \tag{8}
\end{aligned}$$

where in the last term we see the exchange interaction in the Wigner form.

The evolution equation (4) describes the evolution of the electrons in the mean-field approximation for all scale lengths. We are interested in the semiclassical limit where the potential  $\phi$  and the distribution function  $f$  vary on a scale  $L$  much larger than the de Broglie scale length  $\Lambda_{\text{dB}}$  and would like to only keep the lowest surviving correction in an expansion in  $\Lambda_{\text{dB}}/L$ . For the potential term the expansion is straightforward,

see for example Ref. [1]. For the exchange term we expand the potential and the distribution function to second order in  $\mathbf{y}$  (with the assumptions that the characteristic length scale  $L$  is much larger than the thermal de Broglie wave length  $\hbar/mv_T$ , where  $v_T$  is the thermal speed). We then perform the  $\mathbf{y}$ -integration and one of the momentum integrals.

Furthermore, we will for simplicity also assume that the distribution function is independent of the spin, i.e.  $f(\mathbf{x}, \mathbf{p}, \mathbf{s}, t) = f(\mathbf{x}, \mathbf{p}, t)/(4\pi)$ . Integrating over the spin we obtain

$$\begin{aligned}
& \partial_t f(\mathbf{x}, \mathbf{p}, t) + \frac{\mathbf{p}}{m} \cdot \nabla_{\mathbf{x}} f(\mathbf{x}, \mathbf{p}, t) + e\mathbf{E}(\mathbf{x}, t) \cdot \nabla_{\mathbf{p}} f(\mathbf{x}, \mathbf{p}, t) = \frac{1}{2} \partial_p^i \int d^3 r d^3 p' e^{-i\mathbf{r} \cdot \mathbf{p}'/\hbar} [\partial_r^i V(\mathbf{r})] f\left(\mathbf{x} - \frac{\mathbf{r}}{2}, \mathbf{p} + \frac{\mathbf{p}'}{2}, t\right) f\left(\mathbf{x} - \frac{\mathbf{r}}{2}, \mathbf{p} - \frac{\mathbf{p}'}{2}, t\right) \\
&\quad - \frac{i\hbar}{8} \partial_p^i \partial_p^j \cdot \int d^3 r d^3 p' e^{-i\mathbf{r} \cdot \mathbf{p}'/\hbar} [\partial_r^i V(\mathbf{r})] \left[ f\left(\mathbf{x} - \frac{\mathbf{r}}{2}, \mathbf{p} - \frac{\mathbf{p}'}{2}, t\right) \left( \overleftarrow{\partial}_x^j - \overrightarrow{\partial}_x^j \right) f\left(\mathbf{x} - \frac{\mathbf{r}}{2}, \mathbf{p} + \frac{\mathbf{p}'}{2}, t\right) \right] \tag{9}
\end{aligned}$$

where  $\partial_x^i \equiv \partial/\partial x_i$  and analogously for  $\partial_p^i$  and an arrow above

an operator shows which direction it acts. We have also

used the summation convention, so that repeated indices are summed over.

We now consider the effect of the exchange term on electrostatic ion-acoustic waves in a plasma. We will use Eq. (9) for the electrons and the classical Vlasov equation for ions. To obtain the dispersion relation we assume a longitudinal oscillation  $f = f_0(p) + f_1(\mathbf{p})\exp(-i\omega t + ikz)$  and  $\mathbf{E} = \hat{\mathbf{z}}E_z\exp(-i\omega t + ikz)$ . We assume that the unperturbed electron distribution function is given by a Maxwell-Boltzmann distribution [30]

$$f_0(\mathbf{p}) = \frac{n}{(2\pi m k_B T_e)^{3/2}} \exp\left(-\frac{p_\perp^2 + p_z^2}{2m k_B T_e}\right). \quad (10)$$

Furthermore, assuming that the exchange terms are small correction to the distribution function, we may calculate it by in-

serting the lowest order solution for  $f_1$  in the integrand. Introducing spatial spherical coordinates, it is possible to solve all spatial integrals if one assumes that the integrand vanishes in the limit  $r \rightarrow \infty$ . Next, the integrand is expanded in terms of  $\hbar$ . The lowest order term in the first integral vanishes due to symmetry and we keep only the two first order terms. In the second integral we already have an additional  $\hbar$ , meaning that we only retain the lowest order term. Finally it is possible to solve the  $p'_z$  and  $\phi'_p$  integrals. The remaining integrals are solved numerically and doing so gives a solution for  $f_1$  in the linear regime. Now, from the classical dispersion relation we have

$$\omega \approx (\omega_{pI}/\omega_{pe})k v_{Te} \equiv \alpha k v_{Te}, \quad (11)$$

where  $v_{Te} = \sqrt{k_B T_e/m_e}$  is the electron thermal velocity. The dispersion relation is then given by

$$0 = 1 + \frac{\omega_{pe}^2}{k^2 v_{Te}^2} - \frac{\omega_{pI}^2}{\omega^2} - \frac{\hbar^2 \omega_{pe}^4}{4\pi m^2 k^2 v_{Te}^6} \int dv \frac{e^{-v^2}}{(\alpha - v)^2} \int du \left[ \frac{v+u}{\alpha - (v+u)} \right] \left[ \left( u^2 - \frac{u}{\alpha - v} - \frac{1}{2} \right) \text{ExpInt}(-u^2) + e^{-u^2} \right], \quad (12)$$

where the first three terms gives the classical dispersion relation for an ion-acoustic wave. Solving these integrals numerically gives the approximate dispersion relation

$$0 \approx 1 + \frac{\omega_{pe}^2}{k^2 v_{Te}^2} \left( 1 + \frac{2i\gamma_{cl}}{k c_s} \right) - \frac{\omega_{pI}^2}{\omega^2} - \frac{\hbar^2 \omega_{pe}^4}{m^2 k^2 v_{Te}^6} (0.8 + 0.05i).$$

which in the quasi-neutral limit  $\omega_{pe}^2 \gg k^2 v_{Te}^2$  can be written

$$\omega = k c_s \left( 1 + 0.8 \frac{\hbar^2 \omega_{pe}^2}{m^2 v_{Te}^4} \right) - i\gamma_{cl} \left( 1 - 3 \frac{\hbar^2 \omega_{pe}^2}{m^2 v_{Te}^4} \right) \quad (13)$$

where  $c_s = (m_e/m_i)^{1/2} v_{Te}$  is the classical ion-acoustic velocity and we have introduced the classical electron Landau damping,  $\gamma_{cl} = k c_s \sqrt{\pi/8} \sqrt{m_e/m_i}$ , in the cold ion limit [31]. Thus we note that the effective ion-acoustic velocity is *increased*, whereas the damping due to wave-particle interaction is *decreased* due to the exchange effect. As seen from (13) the relative magnitude of both these effects is of the order  $H^2$ , where  $H = \hbar \omega_{pe}/m v_{Te}^2$ . As is shown in, e.g., Ref. [1], plotting the line  $H = 1$  in a log-log density temperature diagram divides the parameter space in a classical regime ( $H \ll 1$ ) and a strong quantum regime ( $H \gtrsim 1$ ). However, such plots are typically performed in order to illustrate the relative importance of particle dispersive effects. Within a kinetic formalism particle dispersion is described by the terms with higher order momentum and spatial derivatives in the Wigner equation [1]. For such terms to be important, in addition to the parameter  $H$  not being too small we also require the macroscopic scale lengths under study to be short. Specifically we need the scale lengths to approach the thermal de Broglie wavelength or shorter. Thus if we exclude the regime of short scale

lengths, as we have done here, the quantum effect of particle dispersion is guaranteed to be of little significance. By contrast, we see that exchange effects may very well affect the long scale behavior of the low-frequency density dynamics. Of particular interest is the change in the damping term. By approaching the regime  $H \sim 1$ , Eq. (13) suggests that we may more or less completely suppress Landau damping of ion-acoustic waves. Physically this makes sense, as classically the particles that are resonantly accelerated for a long time are rather well localized in phase space, which is then counteracted by the exchange terms. Strictly speaking, the regime  $H \sim 1$  does not fit into the perturbation scheme that we have applied here, but qualitatively we still expect this result to be valid.

An important result from this study is the general expression for the exchange term, as given by Eq. (9). This term can describe exchange modification of any type of processes, e.g. altering the coefficients for three-wave interaction [32, 33], adjusting the Zakharov equations [34, 35] or modifying nonlinear wave particle interaction processes [36, 37]. The main restriction is due to the assumption of electrostatic fields. The complexity of the exchange interaction term in (9) in practice forces one to do perturbative calculations. Since the present formalism captures the full effect of a distribution function which may be far from equilibrium, it provides a valuable opportunity to evaluate approaches that relies on other types of approximations. Specifically, in time-dependent density functional theory (TDDFT) [38] the properties of the system is derived from the electron density only (or is at least limited to macroscopic quantities), in which case the full dependence on the detailed momentum distribution is disregarded. Due to the

complexity of many nonlinear plasma systems, such a drastic simplification may be needed, but at the same time it is essential that the accuracy of the approach can be evaluated. Results from DFT calculations have been used to describe electrostatic waves in plasmas, see e.g. Eq. (6) of Ref. [39], where the further approximation of the adiabatic local density approximation (ALDA) has been used. However, a difference with our case is that the Fermi temperature was assumed to be higher than the plasma temperature in these papers. In a very rough sense the previous results agree with ours, as the relative importance of the exchange term scale as  $(\hbar\omega_p/E_K)^2$  in both cases, noting that the characteristic kinetic energy  $E_k$  is the thermal energy  $k_B T$  in our case and the Fermi energy  $k_B T_F$  in the case of Ref. [39]. However, in our case the phase velocity of the ion-acoustic waves is increased due to the exchange interaction, whereas based on Eq. (6) of Ref. [39] the phase velocity is decreased. Still the interpretation of this fact can be debated. One possibility is that the approximation of ALFA to evaluate the exchange potential is too restrictive to capture the ion-acoustic dynamics accurately. Another possibility is that the results are indeed sensitive to the ordering of  $T$  and  $T_F$ , such that the sign of the exchange effect is reversed when the ordering is changed. Regardless of this, it is clear that DFT calculations in general cannot capture the effects of wave-particle interaction, which is responsible for the wave damping in our case.

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